

Generalized tensor methods and entanglement measurements for electronic structure calculations

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In the past decade, we have witnessed a breakthrough in electronic structure calculations due to the density matrix renormalization group (DMRG) method invented by S. R. White [1,2] which has become in recent years a rival to the conventional multiconfiguration wave function approaches [3-5]. Inclusion of the concepts of entanglement from quantum information theory (QIT) [6,7] has paved the road for identifying highly correlated molecular orbitals leading to an efficient construction of active spaces [6,8] and for characterizing the various types of correlation effects relevant for chemical bonding [9]. Quite recently, a reformulation of DMRG in terms of so-called matrix product states (MPS) has shown that it is only one special case in a much more general set of methods: the so-called tensor network states (TNS) [10], which is expected to even outperform DMRG in the near future [11].

In this contribution, we will discuss the quantum chemistry version of the DMRG and tree-TNS algorithms and their applications to transition metal complexes [12] and polydiacetylenes [13]. In the latter case, the state of the art matrix-product-based algorithms is demonstrated by correlating 100 electrons on 100 orbitals allowing us to reproduce experimentally measured quantities with high accuracy. We identify optically dark in-gap states in the singlet and triplet sectors for the first time as seen in experiments.

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